

# Romit Maulik

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## Research interests

Computational fluid dynamics, dynamical systems, scientific machine learning, reduced-order modeling, numerical methods, high-performance computing.

## Positions held

### **January 2026 - Present**

Assistant Professor and Perry Faculty Academic Excellence Scholar, School of Mechanical Engineering, Purdue University.

### **July 2023 - December 2025**

Assistant Professor & Institute of Computational and Data Sciences Co-Hire, Information Sciences and Technology, Pennsylvania State University

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Joint Appointment, Mathematics and Computer Science Division, Argonne National Laboratory.

### **Jun, 2021 - Jun 2023**

Assistant Computational Scientist, Mathematics and Computer Science, Argonne National Laboratory.

### **Oct, 2020 - Jun 2023**

Research Assistant Professor, Department of Applied Mathematics, IIT-Chicago.

### **Jun, 2019 - May, 2021**

Margaret Butler Postdoctoral Fellow, Leadership Computing Facility, Argonne National Laboratory.

### **Jan, 2019 - May, 2019**

Predocctoral Appointee - Mathematics and Computer Science Division, Argonne National Laboratory.

### **Jan, 2016 - Jan, 2019**

Research Assistant - Computational Fluid Dynamics Laboratory, Oklahoma State University.

### **Aug, 2013 - Jul, 2015**

Research Assistant - Computational Biomechanics Laboratory, Oklahoma State University.

### **Jan, 2013 - Dec, 2018**

Teaching Assistant (Introductory Dynamics, Introductory Fluid Mechanics, Practical CFD) - Mechanical & Aerospace Engineering, Oklahoma State University.

### **Aug, 2012 - Aug, 2013**

Design Engineer - Tata Technologies Limited, India.

## Education

PhD. Mechanical & Aerospace Engineering, Oklahoma State University.	<b>2016-2019</b>
M.S. Mechanical & Aerospace Engineering, Oklahoma State University.	<b>2013-2015</b>
B.E. Mechanical Engineering, Birla Institute of Technology, India.	<b>2008-2012</b>

## Honors & awards

ASME Rising Star of Mechanical Engineering, 2026.

Perry Scholar of Academic Excellence, Purdue University, 2026-2031.

Best paper award, CASML IISC Bangalore, 2024, "Improved deep learning of chaotic dynamical systems with multistep penalty losses".

Young Investigator Award, Army Research Office, 2024-2027.

R&D 100 Award Finalist for DeepHyper: An open-source software package for automated and scalable deep learning architecture design.

Best paper award, May 2024, ICLR 2024 Workshop on Climate Change and AI: 'Scaling transformer neural networks for skillful and reliable medium-range weather forecasting'.

Impact Argonne Award, September 2023: 'For developing an AI model for climate and creating an innovated data assimilation methodology'.

Best paper award - Machine Learning-Enabled Prediction of Transient Injection Map In Automotive Injectors With Uncertainty Quantification, 2021 ASME Internal Combustion Engine Fall Conference, <https://doi.org/10.1115/ICEF2021-67888>.

Impact Argonne Award, September, 2021: 'For tackling several climate model challenges and advancing the field of downscaled climate modeling and impact analysis'.

Editor's pick - Reduced-order modeling of advection-dominated systems with recurrent neural networks and convolutional autoencoders , *Physics of Fluids*, <https://doi.org/10.1063/5.0039986>.

Editor's pick - Non-autoregressive time-series methods for stable parametric reduced-order models , *Physics of Fluids*, <https://doi.org/10.1063/5.0019884>.

Margaret Butler Fellow, Argonne Leadership Computing Facility, Argonne National Laboratory, 2019-2021.

SIAM Travel Grant: 2019 SIAM Conference on Computational Science and Engineering, Spokane, WA, 2019.

Outstanding Graduate Student, College of Engineering Architecture and Technology, Oklahoma State University, 2018.

Graduate College Robberson Summer Research Fellowship, Oklahoma State University, 2018.

SIAM TX-LA Section Travel Grant, Texas Applied Mathematics and Engineering Symposium, 2017.

Graduate Student Travel Grant, American Physical Society - Division of Fluid Dynamics, 2017.

Graduate Student Travel Grant, Graduate Program Student Government Authority, Oklahoma State University, 2017.

FGSA Travel Grant for Excellence in Graduate Research, American Physical Society, 2017.

John Brammer Fellowship, Oklahoma State University, 2016.

Graduate College Top Tier Fellowship, Oklahoma State University, 2016.

## Funded Projects

(Active, 2026) Multifidelity data assimilation for improved subgrid and wall-modeling in large eddy simulations of hypersonic flows, ONR, Role: PI.

(Active, 2026) Integrating Graph Neural Operator with MOOSE Framework for Enhanced Transient Modeling and Real-Time Data Assimilation, DOE NEUP, Role: Institutional PI.

(Active, 2026) Diffusion posterior sampling with multimodal language models for adaptive sensor and model fusion, DARPA, Role: PI.

(2027) Workshop Grant: 'Scientific Machine Learning Meets Uncertainty Quantification', National University of Singapore, Institute for Mathematical Sciences, Role: Co-organizer.

(Active, 2026-2030) MURI: Probabilistic Multiscale Inference of Interface Models under Extreme Conditions, Army Research Office, Role: Institutional PI.

(Active, 2025-2027) Synthetic Weather Analogs for DoD Exercises, Training, and Simulation, U.S. Air Force SBIR, Role: Co-PI.

(Active, 2025-2027) Extending the Analog Ensemble Method for Satellite Observations, U.S. Army STTR, Role: Co-PI.

(Active, 2025-2027) Machine learning to improve cycling and forecasts with GEOS and expedite the evaluation of assimilating observations from new instruments, AIST Earth System Digital Twin Award, NASA, Role: PI.

(Active, 2024-2026) Black hole tomography with gravitational waves and artificial intelligence, New Initiative Grant, Charles E. Kaufman Foundation, Role: Co-PI.

(Active, 2024-2027) EARLY CAREER PROGRAM: RIFLES: Rapid Information Fusion through Learning Effective ClosureS, Army Research Office (Modeling of Complex Systems), Role: PI.

(Active, 2024-2027) Using Machine Learning to Uncover Deep Convective Cloud Processes with TRACER Observations, U.S. Department of Energy (Atmospheric System Research), Role: Co-PI.

(Active, 2023-2026) DeepFusion Accelerator for Fusion Energy Sciences in Disruption Mitigations, U.S. Department of Energy (Fusion Energy Sciences), Role: Institutional PI.

(Active, 2024-2026) Foundation models for surface hydrology, Argonne National Laboratory Subaward. Role: Institutional PI.

(Finished, 2021-2025) Inertial neural surrogates for stable dynamical prediction, U.S. Department of Energy (Advanced Scientific Computing Research), Role: Institutional PI.

(Finished, 2020-2025) RAPIDS2: A SciDAC Institute for Computer Science, Data, and Artificial Intelligence, U.S. Department of Energy (Advanced Scientific Computing Research). Role: Senior Personnel.

(Finished, 2021-2023) AI emulator assisted data assimilation, Future computing, LDRD-Prime, Argonne National Laboratory, U.S. Department of Energy. Role: Co-PI (Argonne National Laboratory).

(Finished, 2022-2023) A Scalable, Energy Efficient HPC Environment for AI-Enabled Science, National Science Foundation Collaborative PPOSS funding. Role: Co-PI (IIT-Chicago).

(Finished, 2021) SambaWF: Highly resolved surrogate models for weather forecasting, LDRD-Expedition, Argonne National Laboratory, U.S. Department of Energy. Role: PI (Argonne National Laboratory).

(Finished, 2019-2021) Scalable machine learning for turbulence closure and reduced-order modeling, Margaret Butler Fellowship, Role: PI (Argonne National Laboratory).

## Compute Allocations

(Active, 2025-) Scientific machine learning for fluid dynamics surrogate modeling and multiscale data recovery, AI4Science Compute Allocation, Perlmutter, NERSC.

(Active, 2023-) Neural differential equations for scientific discovery, Director's Discretionary Allocation, Polaris, Argonne National Laboratory.

(Active, 2025-) Probabilistic machine learning models for unstructured fluid dynamics data, Director's Discretionary Allocation, Aurora, Argonne National Laboratory.

## Supervision

Asterisks indicate active supervision.

Dr. Sourajit Das\*, Postdoctoral Scholar, Pennsylvania State University, 2025-Present.

Dr. Melissa Adrian\*, Lillian Gilbreth Postdoctoral Fellow, Purdue University, 2026-Present.

Dr. Yang Xu\*, Postdoctoral Scholar, Purdue University, 2026-Present.

Dr. Sen Wang\*, Postdoctoral Scholar, Purdue University, 2026-Present.

Dibyajyoti Chakraborty\*, PhD Student, Pennsylvania State University, 2023-Present.

Haiwen Guan\*, PhD Student, Pennsylvania State University, 2024-Present.

Hojin Kim\*, PhD Student, Purdue University, 2024-Present.

Ashwin Suriyanarayan\*, PhD Student, Pennsylvania State University, 2025-Present.

Kanad Sen\*, PhD Student, Purdue University, 2026-Present.

Dr. James Henry, Postdoctoral Scholar, Pennsylvania State University, 2024-2026 (Next position - Senior Propulsion Design Engineer - Astro Mechanica).

Dr. Shivam Barwey, AETS Named Postdoctoral Fellow, Argonne National Laboratory, 2022-2025 (Next position - tenure-track faculty at University of Notre Dame).

Dr. Xuyang Li, Postdoctoral Scholar, Pennsylvania State University, 2024-2025 (Next position - tenure-track faculty at UNC-Charlotte).

Dr. Matthew Poska, PhD Student, Pennsylvania State University & Argonne National Laboratory. DOE SCGSR Fellow, 2022-2025 (co-advised with Prof. Sharon Huang, IST, Penn State, next position - Engineer at Pinterest).

Zachariah Malik, Visiting graduate Student, Argonne National Laboratory, NSF MSGI Fellow, Summer 2023, 2024 (Next position - PhD candidate at CU Boulder).

Vinamr Jain, Undergraduate Intern, IIT-Delhi, 2023-2024 (Next position - PhD student at Cornell University).

Aaryan Bavishi, Undergraduate Student, Pennsylvania State University, 2023-2024 (Next position - Analyst at FNB Corp).

Abhinab Bhattacharjee, Graduate Student, Argonne National Laboratory, Givens Associate, Summer 2023 (Next position - PhD candidate at Virginia Tech).

Deepinder Jot Singh Aulakh, Graduate Student, Argonne National Laboratory, ALCF Research Aide, Summer 2023 (Next position - Software Developer at Symmetry).

Trent Gerew, Undergraduate Student, Argonne National Laboratory, DOE SULI Program, Spring 2023 (Next position - PhD student at the University of Kansas).

Jonah Botvinick-Greenhouse, Visiting Graduate Student, Cornell University & Argonne National Laboratory, NSF MSGI Fellow, Summer 2022 (Next position - PhD candidate at Cornell University).

Sen Lin, Graduate Student, Argonne National Laboratory, Givens Associate, Summer 2022 (Next position - PhD candidate at University of Houston).

Cyril Le Doux, Undergraduate Student, Argonne National Laboratory, DOE SULI Program, Summer 2022 (Next position - Undergraduate at UChicago).

Gurpreet Singh Hora, Graduate Student, Summer 2022 (With Laurent White at AMD Research, Next position - PhD student at Columbia University).

Sahil Bhola, Graduate Student, Argonne National Laboratory, ALCF Research Aide, Summer 2021 (Next position - PhD student at University of Michigan).

Alec Linot, Graduate Student, Argonne National Laboratory, Givens Associate, Summer 2021 (Next position - PhD student at the University of Wisconsin).

Janah Richardson, High-school student, Afro-Academic, Cultural, Technological and Scientific Olympics (ACT-SO) High School Research Program, 2020-2021. Gold medal winner in Computer Science category-Illinois.

Suraj Pawar, Graduate Student, Argonne National Laboratory, ALCF Research Aide, Summer 2020 (Next position - PhD candidate at Oklahoma State University).

Dominic Skinner, Graduate Student, Argonne National Laboratory, NSF MSGI Fellow, Summer 2020 (Next position - PhD student at MIT).

## Publications

### *Under review*

1. A. Suriyanarayanan, D. Chakraborty, M. Adrian, **R. Maulik**, Deep Learning of Solver-Aware Turbulence Closures from Nudged LES Dynamics, *arXiv:2604.23874*.

2. D. Chakraborty, H. Kim, **R. Maulik**, Adaptive Diffusion Posterior Sampling for Data and Model Fusion of Complex Nonlinear Dynamical Systems, *arXiv:2603.12635*.
3. H. Guan, M. Darmian, D. Chakraborty, T. Arcomano, A. Chattopadhyay, **R. Maulik**, High-Resolution Climate Projections Using Diffusion-Based Downscaling of a Lightweight Climate Emulator, *arXiv:2602.13416*.
4. S. Das, D. Chakraborty, **R. Maulik**, SC<sub>3</sub>D: Dynamic and Differentiable Causal Discovery for Temporal and Instantaneous Graphs, *Arxiv:2602.02830*.
5. X. Li, J. Harlim, **R. Maulik**, A Weak Penalty Neural ODE for Learning Chaotic Dynamics from Noisy Time Series, *Arxiv:2511.06609*.
6. D. Chakraborty, **R. Maulik**, P. Harrington, D. Foster, M. Nabian, S. Choudhry, MoWE : A Mixture of Weather Experts, *Arxiv: 2509.09052*
7. H. Guan, T. Arcomano, A. Chattopadhyay, **R. Maulik**: LUCIE-3D: A three-dimensional climate emulator for forced responses, *Arxiv: 2509.02061*.
8. H. Kim, V. Shankar, V. Vishwanathan, **R. Maulik**: Generalizable data-driven turbulence closure modeling on unstructured grids with differentiable physics, *arXiv:2307.13533*.
9. R. Rawat, **R. Maulik**, S. Barwey: FIGNN: Feature-Specific Interpretability for Graph Neural Network Surrogate Models *arXiv:2506.11398*.

### Peer-reviewed journal articles

You can find virtually ever paper below on the Arxiv. If you cannot, please email me for a copy.

1. X. Li, **R. Maulik**: SALSA-RL: Stability Analysis in the Latent Space of Actions for Reinforcement Learning, *Neural Networks*, Volume 201, 108957, 2026.
2. D. Chakraborty, A. Mohan, **R. Maulik**: Binned Spectral Power Loss for Improved Prediction of Chaotic Systems, *Journal of Computational Physics*, Volume 558, 114866, 2026.
3. X. Wang, J. Yang, J. Adie, K. Furtado, C. Chen, T. Arcomano, **R. Maulik**, G. Mengaldo: CondensNet: Enabling stable long-term climate simulations via hybrid deep learning models with adaptive physical constraints, *npj Climate and Atmospheric Science*, 9 (1), 7, 2026.
4. D. Chakraborty, H. Guan, J. Stock, T. Arcomano, G. Cervone, **R. Maulik**: Multimodal atmospheric super-resolution with deep generative models, *Machine Learning: Earth*, Volume 2, 015001, 2025.
5. J. Botvinick-Greenhouse, M. Oprea, **R. Maulik**, Y. Yang: Measure-Theoretic Time-Delay Embedding: Analysis and Application, *Journal of Statistical Physics*, 192 (12), 171, 2025.
6. H. Guan, T. Arcomano, A. Chattopadhyay, **R. Maulik**: LUCIE: A Lightweight Uncoupled Climate Emulator with long-term stability and physical consistency, *Journal of Advances in Modeling Earth Systems*, Volume 17, Issue 11, 2025.
7. S. Barwey, P. Pal, S. Patel, R. Balin, B. Lusch, V. Vishwanath, **R. Maulik**, R. Balakrishnan: Mesh-based Super-Resolution of Fluid Flows with Multiscale Graph Neural Networks, *Computer Methods in Applied Mechanics and Engineering*, Volume 443, 1 August 2025, 118072.
8. A. Nair, S. Barwey, P. Pal, J. MacArt, **R. Maulik**: Understanding Latent Timescales in Neural Ordinary Differential Equation Models for Advection-Dominated Dynamical Systems, *Physica D: Nonlinear Phenomena*, 134650, 2025.

9. Z. Malik, **R. Maulik**: A competitive baseline for deep learning enhanced data assimilation using conditional Gaussian ensemble Kalman filtering, *Computer Methods in Applied Mechanics and Engineering*, 440, 117931, 2025.
10. V. Shankar, D. Chakraborty, V. Vishwanathan, **R. Maulik**: Differentiable turbulence: Closure as PDE-constrained optimization, *Physical Review Fluids*, 10, 024605, 2025.
11. T. Chang, A. Gillette, **R. Maulik**: Leveraging Interpolation Models and Error Bounds for Verifiable Scientific Machine Learning, *Journal of Computational Physics*, Volume 524, 1 March 2025, 113726.
12. S. Barwey, H. Kim, **R. Maulik**: Interpretable A-posteriori Error Indication for Graph Neural Network Surrogate Models, *Computer Methods in Applied Mechanics and Engineering*, Volume 433, Part B, 1 January 2025, 117509.
13. D. Chakraborty, S. Chung, **R. Maulik**: Divide and conquer: Learning chaotic dynamical systems with multistep penalty neural ordinary differential equations, *Computer Methods in Applied Mechanics and Engineering*, Volume 432, Part A, 1 December 2024, 117442.
14. B. Sanderse, P. Stinis, **R. Maulik**, S. Ahmed: Scientific machine learning for closure models in multiscale problems: a review, *Foundations of Data Science*, 2024.
15. C. Moss, **R. Maulik**, V. Iungo: Augmenting Insights from Wind Turbine Data through Data-Driven Approaches, *Applied Energy*, 376, 124116, 2024.
16. D. Aulakh, X. Yang, **R. Maulik**: Robust experimental data assimilation for the Spalart-Allmaras turbulence model, *Physical Review Fluids*, 9, 084608, 2024.
17. S. Yang, H. Kim, Y. Hong, K. Yee, **R. Maulik**, N. Kang: Data-driven Physics-Informed Neural Networks: A Digital Twin Perspective, *Computer Methods in Applied Mechanics and Engineering*, Volume 428, 117075, 2024.
18. M. Rogowski, B. Yeung, O. Schmidt, **R. Maulik**, M. Parsani, L. Dalcin, G. Mengaldo: Unlocking massively parallel spectral proper orthogonal decompositions in the PySPOD package, *Computer Physics Communications*, Volume 302, 109246, 2024.
19. K. Asztalos, R. Steijl, **R. Maulik**: Reduced-order modeling on a near-term quantum computer, *Journal of Computational Physics*, Volume 510, 113070, 2024.
20. C. Moss, **R. Maulik**, G. Iungo: A Call for Enhanced Data-Driven Insights into Wind Energy Flow Physics, *Theoretical and Applied Mechanics Letters*, Volume 14, Issue 1, 2024, 100488.
21. S. Barwey, V. Shankar, V. Vishwanathan, **R. Maulik**: Multiscale graph neural network autoencoders for interpretable scientific machine learning, *Journal of Computational Physics*, Volume 495, 15 December 2023, 112537.
22. C. Moss, M. Puccioni, **R. Maulik**, C. Jacquet, D. Apgar, G. V. Iungo : Predicting Wind Farm Operations with Machine Learning and the P2D-RANS model: A Case Study for an AWAKEN Site, *Wind Energy*, 2023.
23. S. Lin, G. Mengaldo, **R. Maulik**: Online data-driven changepoint detection for high-dimensional dynamical systems, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 33, 10, 2023.
24. J. Botvinick-Greenhouse, Y. Yang, **R. Maulik**: Generative Modeling of Time-Dependent Densities via Optimal Transport and Projection Pursuit, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 33, 10, 2023.

25. C. Jang, J. Choi, **R. Maulik**, D. Lim: Determinants of Adult Education and Training Participation in the United States: A Machine Learning Approach, *Adult Education Quarterly*, 2023.
26. **R. Maulik**, R. Egele, K. Raghavan, P. Balaprakash: Quantifying uncertainty for deep learning based forecasting and flow-reconstruction using neural architecture search ensembles, *Physica D.*, 454, 133852, 2023.
27. A. Aygun, **R. Maulik**, A. Karakus: Physics-Informed Neural Networks for Mesh Deformation with Exact Boundary Enforcement, *Engineering Applications of Artificial Intelligence*, 125, 106660, 2023.
28. S. Bhola, S. Pawar, P. Balaprakash, **R. Maulik**: Multi-fidelity reinforcement learning framework for shape optimization, *Journal of Computational Physics*, 482, 112018, 2023.
29. V. Shankar, V. Puri, R. Balakrishnan, **R. Maulik**, V. Vishwanathan: Differentiable physics-enabled closure modeling for Burgers' turbulence, *Machine Learning Science and Technology*, 4, 015017, 2023.
30. J. Choi, W. Wehde, **R. Maulik**: Politics of Problem Definition: Comparing Public Support of Climate Change Mitigation Policies using Machine Learning, *Review of Policy Research*, 2022.
31. S. Mondal, G. Magnotti, B. Lusch, **R. Maulik**, R. Torelli: Machine Learning-Enabled Prediction of Transient Injection Map in Automotive Injectors With Uncertainty Quantification, *Journal of Engineering for Gas Turbines and Power*, 145(4), 041015, 2023
32. A. Linot, J. Burby, Q. Tang, P. Balaprakash, M. Graham, **R. Maulik**: Stabilized Neural Ordinary Differential Equations for Long-Time Forecasting of Dynamical Systems, *Journal of Computational Physics*, 474, 111838, 2022.
33. N. Garland, **R. Maulik**, Q. Tang, X. Tang, P. Balaprakash, Efficient training of artificial neural network surrogates for a collisional-radiative model through adaptive parameter space sampling, *Machine Learning Science and Technology*, 3 (4), 045003, 2022.
34. M. Morimoto, K. Fukami, **R. Maulik**, R. Vinuesa, K. Fukagata: Assessments of model-form uncertainty using Gaussian stochastic weight averaging for fluid-flow regression, *Physica D: Nonlinear Phenomena*, 133454, 2022.
35. A. Lario, **R. Maulik**, G. Rozza, G. Mengaldo: Neural-network learning of SPOD dynamics, *Journal of Computational Physics*, 111475, 2022.
36. G. Iungo, **R. Maulik**, S. Renganathan, S. Letizia: Machine-learning identification of the variability of mean velocity and turbulence intensity for wakes generated by onshore wind turbines: Cluster analysis of wind LiDAR measurements, *Journal of Renewable and Sustainable Energy*, 14 (Cover article), 023307, 2022.
37. **R. Maulik**, V. Rao, J. Wang, G. Mengaldo, E. Constantinescu, B. Lusch, P. Balaprakash, I. Foster, R. Kotamarthi, Efficient high-dimensional variational data assimilation with machine-learned reduced-order models, *Geoscientific Model Development*, 15, 3433–3445, 2022..
38. Y. Lu, **R. Maulik**, T. Gao, F. Dietrich, I. Kevrekidis, J. Duan: Learning the temporal evolution of multivariate densities via normalizing flows, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 32 (3), 033121, 2022.
39. **R. Maulik**, D. Fytanidis, B. Lusch, S. Patel, V. Vishwanath: PythonFOAM: In-situ data analyses with OpenFOAM and Python, *Journal of Computational Science*, 62, 101750, 2022.
40. S. Renganathan, **R. Maulik**, G. Iungo, S. Letizia: Data-driven wind turbine wake modeling using probabilistic machine learning, *Neural Computing and Applications*, 34, 6171–618, 2022.

41. K. Lyras, **R. Maulik**, D. Schmidt: Machine-learning accelerated turbulence modelling of transient flashing jets, *Physics of Fluids*, 33, 127104 (2021).
42. K. Fukami, **R. Maulik**, N. Ramachandra, K. Taira, K. Fukagata: Global field reconstruction from sparse sensors with Voronoi tessellation-assisted deep learning, *Nature Machine Intelligence*, 2021.
43. B. Hamzi, **R. Maulik**, H. Owhadi: Simple, low-cost, and accurate, data-driven geophysical forecasting with learned kernels, *Proceedings of the Royal Society A*, 477: 20210326, 2021.
44. G. Mengaldo, **R. Maulik**, PySPOD: A Python package for Spectral Proper Orthogonal Decomposition (SPOD), *Journal of Open Source Software*, 6 (6), 2862, 2021.
45. **R. Maulik**, B. Lusch, P. Balaprakash: Reduced-order modeling of advection-dominated systems with recurrent neural networks and convolutional autoencoders, *Physics of Fluids*, 33, 037106, 2021.
46. S. Pawar, **R. Maulik**: Distributed deep reinforcement learning for simulation control, *Machine Learning: Science and Technology*, 2, 025029, 2021.
47. S. Renganathan, **R. Maulik**, J. Ahuja: Enhanced data efficiency using deep neural networks and Gaussian processes for aerodynamic design optimization, *Aerospace Science and Technology*, 111, 106522, 2021.
48. J. Burby, Q. Tang, **R. Maulik**: Fast neural Poincaré maps for toroidal magnetic fields, *Plasma Physics and Controlled Fusion*, 63, 024001, 2021.
49. **R. Maulik**, T. Botsas, N. Ramachandra, M. Lachlan, I. Pan: Latent-space time evolution of non-intrusive reduced-order models using Gaussian process emulation, *Physica D: Nonlinear Phenomena*, 132797, 2021.
50. **R. Maulik**, H. Sharma, S. Patel, B. Lusch, E. Jennings : A turbulent eddy-viscosity surrogate modeling framework for Reynolds-Averaged Navier-Stokes simulations, *Computers and Fluids*, 104777, 2020.
51. **R. Maulik**, K. Fukami, N. Ramachandra, K. Fukagata, K. Taira : Probabilistic neural networks for fluid flow surrogate modeling and data recovery, *Physical Review Fluids*, 5, 104401, 2020.
52. **R. Maulik**, P. Balaprakash, B. Lusch: Non-autoregressive time-series methods for stable parametric reduced-order models, *Physics of Fluids*, 32, 087115, 2020.
53. **R. Maulik**, N. Garland, X. Tang, P. Balaprakash: Neural network representability of fully ionized plasma fluid model closures, *Physics of Plasmas*, 27, 072106, 2020.
54. J. Choi, S. Robinson, **R. Maulik**, W. Wehde: What Matters the Most for Individual Disaster Preparedness? Understanding Emergency Preparedness Using Machine Learning, *Natural Hazards*, 103, 1183-1200, 2020.
55. S. Renganathan **R. Maulik**, V. Rao : Machine learning for nonintrusive model order reduction of the parametric inviscid transonic flow past an airfoil, *Physics of Fluids*, 32, 047110, 2020.
56. **R. Maulik**, O. San: Numerical assessments of a parametric implicit large eddy simulation model, *Journal of Computational and Applied Mathematics*, 112866, 2020.
57. **R. Maulik**, O. San, J. Jacob: Spatiotemporally dynamic implicit large eddy simulation using machine learning classifiers, *Physica D: Nonlinear Phenomena*, 406, 132409, 2020.
58. **R. Maulik**, A. Mohan, B. Lusch, S. Madireddy, P. Balaprakash, D. Livescu: Time-series learning of latent-space dynamics for reduced-order model closure, *Physica D: Nonlinear Phenomena*, 405, 132368, 2020.

59. Y. Hossain, **R. Maulik**, H. Park, M. Ahmed, C. Bach, O. San: Improvement of Unitary Equipment and Heat Exchanger Testing Methods, *ASHRAE Transactions*, 125.2, 2019.
60. **R. Maulik**, O. San, J. Jacob, C. Crick: Sub-grid scale model classification and blending through deep learning, *Journal of Fluid Mechanics*, 870, 784-812, 2019.
61. O. San, **R. Maulik**, M. Ahmed: An artificial neural network framework for reduced order modeling of transient flows, *Communications in Nonlinear Science and Numerical Simulation*, 77, 271-287, 2019.
62. **R. Maulik**, O. San, A. Rasheed, P. Vedula: Subgrid modeling for two-dimensional turbulence using artificial neural networks, *Journal of Fluid Mechanics*, 858, 122-144, 2019.
63. **R. Maulik**, O. San, A. Rasheed, P. Vedula: Data-driven deconvolution for large eddy simulation of Kraichnan turbulence, *Physics of Fluids*, 30, 125109, 2018.
64. O. San, **R. Maulik**: Stratified Kelvin-Helmholtz turbulence of compressible shear flows, *Nonlinear Processes in Geophysics*, 25, 457-476, 2018.
65. O. San, **R. Maulik**: Extreme learning machine for reduced order modeling of turbulent geophysical flows, *Physical Review E*, 97, 042322, 2018.
66. O. San, **R. Maulik**: Machine learning closures for model order reduction of thermal fluids, *Applied Mathematical Modelling*, 60, 681-710, 2018.
67. **R. Maulik**, O. San, R. Behera : An adaptive multilevel wavelet framework for scale-selective WENO reconstruction schemes, *International Journal of Numerical Methods in Fluids*, 87 (5), 239-269, 2018.
68. O. San, **R. Maulik**: Neural network closure models for nonlinear model order reduction, *Advances in Computational Mathematics*, 44, 1717-1750, 2018.
69. **R. Maulik**, O. San: A dynamic closure modeling framework for large eddy simulation using approximate deconvolution: Burgers equation, *Cogent Physics*, 5, 1464368, 2018.
70. **R. Maulik**, O. San: A neural network approach for the blind deconvolution of turbulent flows, *Journal of Fluid Mechanics*, 831, 151-181, 2017.
71. **R. Maulik**, O. San: A novel dynamic framework for subgrid-scale parametrization of mesoscale eddies in quasigeostrophic turbulent flows, *Computers and Mathematics with Applications*, 74, 420-445, 2017.
72. **R. Maulik**, O. San: Explicit and implicit LES closures for Burgers turbulence, *Journal of Computational and Applied Mathematics*, 327, 12-40, 2017.
73. **R. Maulik**, O. San: Resolution and energy dissipation characteristics of implicit LES and explicit filtering models for compressible turbulence, *Fluids*, 2(2)-14, 2017.
74. **R. Maulik**, O. San: A dynamic subgrid-scale modeling framework for Boussinesq turbulence, *International Journal of Heat and Mass Transfer*, 108, 1656-1675, 2017.
75. **R. Maulik**, O. San: A dynamic framework for functional parameterisations of the eddy viscosity coefficient in two-dimensional turbulence, *International Journal of Computational Fluid Dynamics*, 31(2), 69-92, 2017.
76. **R. Maulik**, O. San: A stable and scale-aware dynamic modeling framework for subgrid-scale parameterizations of two-dimensional turbulence, *Computers & Fluids* 158, 11-38, 2016.
77. **R. Maulik**, O. San: Dynamic modeling of the horizontal eddy viscosity coefficient for quasigeostrophic ocean circulation problems, *Journal of Ocean Engineering and Science* 1, 300-324, 2016.

78. H. H. Marbini, **R. Maulik**: A biphasic transversely isotropic poroviscoelastic model for the unconfined compression of hydrated soft tissue, *Journal of Biomechanical Engineering* 138, 031003, 2016.

### *Peer-reviewed conference publications*

1. X. Wang, J. Yang, J. Adie, K. Furtado, C. Chen, T. Arcomano, **R. Maulik**, G. Mengaldo: CondensNet: Enabling stable long-term climate simulations via hybrid deep learning models with adaptive physical constraints, *AI4X Conference*, Singapore, 2025.
2. H. Zhang, Y. Liu, **R. Maulik**: Semi-Implicit Neural Ordinary Differential Equations, The 39th Annual AAAI Conference on Artificial Intelligence, 2025. <https://openreview.net/forum?id=MeALSxFb5A&noteId=ffoAQc9SLo>
3. D. Chakraborty, S. Chung, A. Chattopadhyay, **R. Maulik**: Improved deep learning of chaotic dynamical systems with multistep penalty losses, *Conference on Applied AI and Scientific Machine Learning*, IISC Bangalore (Spotlight paper < 5%) *arXiv:2410.05572*.
4. T. Nguyen, R. Shah, H. Bansal, T. Arcomano, S. Madireddy, **R. Maulik**, V. Kotamarthi, I. Foster, A. Grover: Scaling transformers for skillful and reliable medium-range weather forecasting, *Neural Information Processing Systems*, 2024
5. R. Egele, **R. Maulik**, K. Raghavan, P. Balaprakash, B. Lusch: AutoDEUQ: Automated Deep Ensemble with Uncertainty Quantification, *26th International Conference on Pattern Recognition*, 1908–1914, 2022.
6. Sudepta Mondal, Gina M. Magnotti, Bethany Lusch, **Romit Maulik**, Roberto Torelli: Machine Learning-Enabled Prediction of Transient Injection Map in Automotive Injectors With Uncertainty Quantification, *ASME Internal Combustion Engine Fall Conference*, 2021.
7. H. Shan, Y. Sun, **R. Maulik**, T. Xu: Application of Artificial Neural Network in the APS LINAC Bunch Charge Transmission Efficiency, *12th International Particle Accelerator Conference (IPAC)*, 2021., <https://accelconf.web.cern.ch/ipac2021/papers/tupab287.pdf>.
8. V. Sastry, **R. Maulik**, V. Rao, B. Lusch, S. Renganathan, R. Kotamarthi: Data-driven deep learning emulators for geophysical forecasting, *International Conference on Computational Science*, 433-446, 2021, [https://doi.org/10.1007/978-3-030-77977-1\\_35](https://doi.org/10.1007/978-3-030-77977-1_35).
9. **R. Maulik**, R. Egele, B. Lusch, P. Balaprakash: Recurrent neural network architecture search for geophysical emulation, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC)*, 2020, 10.5555/3433701.3433711.
10. V. Rao, **R. Maulik**, E. Constantinescu, M. Anitescu: A machine learning method for computing rare event probabilities, *International Conference on Computational Science*, 169-182, 2020, [https://link.springer.com/chapter/10.1007%2F978-3-030-50433-5\\_14](https://link.springer.com/chapter/10.1007%2F978-3-030-50433-5_14).
11. **R. Maulik**, O. San, C. Bach: A computational investigation of the effect of ground clearance in vertical ducting systems, *International High Performance Buildings Conference*, Herrick Laboratories, Purdue University, 2018. <https://docs.lib.purdue.edu/ihpbc/308/>.

### *Conference publications*

1. J. Henry, **R. Maulik**: Surrogate Modeling of Fluidic Oscillator Pairs, *AIAA SciTech Form* 2026 <https://doi.org/10.2514/6.2026-0941>.

2. V. Jain, **R. Maulik**: Higher order quantum reservoir computing for non-intrusive reduced-order models, AIAA SciTech Form 2026, <https://doi.org/10.2514/6.2026-1419>.
3. **R. Maulik**, H. Sharma, S. Patel, B. Lusch, E. Jennings: Deploying deep learning in OpenFOAM with TensorFlow: A tutorial, AIAA SciTech Forum 2021, <https://doi.org/10.2514/6.2021-1485>.
4. P. Milan, R. Torelli, B. Lusch, **R. Maulik**, G. Magnotti: Data-Driven Modeling of Large-Eddy Simulations for Fuel Injector Design, AIAA SciTech Forum 2021, <https://doi.org/10.2514/6.2021-1016>.
5. **R. Maulik**, V. Rao, S. Renganathan, S. Letizia, G. Iungo: Cluster analysis of wind turbine wakes measured through a scanning Doppler wind LiDAR, AIAA SciTech Forum 2021, <https://doi.org/10.2514/6.2021-1181>.

### *Peer-reviewed workshop proceedings*

1. X. Li, M. Masmoudi, R. Gharbi, N. Lajnef, V. Boddetti, J. Harlim, **R. Maulik**: Neural-VSI: Variational System Identification of Structural Parameter Fields in High-Order PDEs, ICLR Workshop on Artificial Intelligence and Partial Differential Equations, 2026, Rio De Janeiro, Brazil.
2. H. Kim, **R. Maulik**: Towards Interpretable Deep Learning and Analysis of Dynamical Systems via the Discrete Empirical Interpolation Method, AAAI Workshop on Explainable AI, Singapore, 2026.
3. X. Li, **R. Maulik**: Reinforcement Learning Stability Analysis in the Latent Space of Actions, AAAI 2025 bridge program on Knowledge-guided Machine Learning, February 25-26, 2025.
4. J. Henry, **R. Maulik**: Reduced complexity modeling of fluidic oscillators with data-driven boundary conditions, AAAI 2025 bridge program on Knowledge-guided Machine Learning, February 25-26, 2025.
5. H. Guan, D. Chakraborty, **R. Maulik**: Atmospheric Super-Resolution with Neural Operators, AAAI 2025 bridge program on Knowledge-guided Machine Learning, February 25-26, 2025.
6. D. Chakraborty, S. W. Chung, A. Chattopadhyay, T. Arcomano, **R. Maulik**: Improved deep learning of chaotic dynamical systems with multistep penalty losses, AAAI 2025 bridge program on Knowledge-guided Machine Learning, February 25-26, 2025.
7. H. Kim, S. Barwey, **R. Maulik**: Scalable, adaptive, and explainable scientific machine learning with applications to surrogate models of partial differential equations, , AAAI 2025 bridge program on Knowledge-guided Machine Learning, February 25-26, 2025.
8. H. Kim, S. Barwey, **R. Maulik**: Scalable, adaptive, and explainable scientific machine learning with applications to surrogate models of partial differential equations, AAAI Symposium on Integrated Approaches to Computational Scientific Discovery, November 7-9, 2024.
9. S. Barwey, R. Balin, B. Lusch, S. Patel, R. Balakrishnan, P. Pal, **R. Maulik**, V. Vishwanath: Scalable and Consistent Graph Neural Networks for Distributed Mesh-based Data-driven Modeling, (Workshop on Machine Learning with Graphs in High Performance Computing Environments), Supercomputing 2024.
10. H. Guan, T. Arcomano, A. Chattopadhyay, **R. Maulik**: LUCIE: A Lightweight Uncoupled Climate Emulator with long-term stability and physical consistency for O(1000)-member ensembles, (Machine Learning for Earth System Modeling Workshop, ICML 2024).

11. T. Nguyen, R. Shah, H. Bansal, T. Arcomano, S. Madireddy, **R. Maulik**, V. Kotamarthi, I. Foster, A. Grover: Scaling transformers for skillful and reliable medium-range weather forecasting, ICLR AI4DiffEqtnsInSci Workshop 2024 (Accepted as spotlight presentation and awarded best paper).
12. A. Nair, S. Barwey, P. Pal, **R. Maulik**: Investigation of Latent Time-Scales in Neural ODE Surrogate Models, ICLR AI4DiffEqtnsInSci Workshop 2024 (Accepted as poster).
13. H. Zhang, Y. Liu, **R. Maulik** Semi-Implicit Neural Ordinary Differential Equations for Learning Chaotic Systems, NeurIPS 2023 Workshop Heavy Tails in Machine Learning, NeurIPS 2023.
14. V. Shankar, S. Barwey, **R. Maulik**, V. Vishwanathan: Practical implications of equivariant and invariant graph neural networks for fluid flow modeling, Physics4ML Workshop, ICLR 2023, <https://openreview.net/forum?id=3Y6XRCIUT5>.
15. **R. Maulik**, G. Mengaldo: PyParSVD: A streaming, distributed and randomized singular-value-decomposition library, (7th International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-7), Supercomputing 2021).
16. D. Skinner, **R. Maulik**: Meta-modeling strategy for data-driven forecasting, *Tackling Climate Change with Machine Learning Workshop, NeurIPS*, 2020. <https://www.climatechange.ai/papers/neurips2020/13.html>.
17. N. Garland, **R. Maulik**, Q. Tang, X. Tang, P. Balaprakash: Progress towards high fidelity collisional-radiative model surrogates for rapid in-situ evaluation, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2020. [https://ml4physicalsciences.github.io/2020/files/NeurIPS\\_ML4PS\\_2020\\_79.pdf](https://ml4physicalsciences.github.io/2020/files/NeurIPS_ML4PS_2020_79.pdf).
18. K. Fukami, **R. Maulik**, N. Ramachandra, K. Fukagata, K. Taira: Probabilistic neural network-based reduced-order surrogate for fluid flows, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2020. [https://ml4physicalsciences.github.io/2020/files/NeurIPS\\_ML4PS\\_2020\\_7.pdf](https://ml4physicalsciences.github.io/2020/files/NeurIPS_ML4PS_2020_7.pdf)
19. **R. Maulik**, R. S. Assary, P. Balaprakash: Site-specific graph neural network for predicting protonation energy of oxygenate molecules, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2019. [https://ml4physicalsciences.github.io/2019/files/NeurIPS\\_ML4PS\\_2019\\_134.pdf](https://ml4physicalsciences.github.io/2019/files/NeurIPS_ML4PS_2019_134.pdf)
20. **R. Maulik**, V. Rao, S. Madireddy, B. Lusch, P. Balaprakash: Using recurrent neural networks for non-linear component computation in advection-dominated reduced-order models, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2019. [https://ml4physicalsciences.github.io/2019/files/NeurIPS\\_ML4PS\\_2019\\_99.pdf](https://ml4physicalsciences.github.io/2019/files/NeurIPS_ML4PS_2019_99.pdf).

## Talks presented

1. How can the differentiable physics paradigm be used without adjoints?, **Invited Talk**, Data-driven Modelling for Mechanical Systems Summer School 2026, IIT (ISM) Dhanbad, July 1, 2026.
2. Nudging-based data assimilation for interpretable scientific machine learning, **Invited Talk**, EuroMech Colloquium on Physics-enhanced machine learning and data-driven nonlinear dynamics, Lake Como, Italy, April 28, 2026.
3. No more adjoints: Calibrating chaotic dynamical systems with weak-form learning, **Invited Talk**, Workshop on Scientific Machine Learning, Korea Institute for Advanced Study, March 26, 2026.
4. Diffusion models as foundations for digital twins, **Invited Talk**, Environmental Fluid Dynamics Seminar Series, The University of Notre Dame, February 3, 2026.

5. Multimodal data and model fusion for high-dimensional dynamical systems, **Invited Talk**, PC-13: Data-Driven Modeling of Combustion Dynamics AIAA 2026 Panel Session, January 2026.
6. Multimodal data and model fusion for the atmosphere using diffusion models, **Invited Talk**, Workshop on Reduced Order and Surrogate Modeling for Digital Twins, IMSI University of Chicago, November 14, 2025.
7. Differentiable Physics: A physics-constrained and data-driven paradigm for scientific machine learning, **Invited Talk**, ASIA-USA Seminar Series, USACM Math Methods in Computational Engineering & Sciences, November 4, 2025.
8. No more adjoints: Calibrating chaotic dynamical systems with weak-form learning, **Invited Talk**, PDE and Applied Mathematics Seminar, UC Riverside, October 29, 2025.
9. Multimodal data and model fusion for the atmosphere using diffusion models, **Invited Talk**, Advanced Modeling and Simulations Seminar Series, Texas A & M University, Kingsville, October 2025.
10. Multimodal data and model fusion for the atmosphere using diffusion models, **Invited Talk**, Penn State University ADAPT Center Seminar Series, September 30, 2025.
11. Scalable, adaptive, and explainable geometric deep learning with applications to computational physics, **Invited talk**, Workshop on Surrogates and Dimension Reduction in Scientific Machine Learning, University of Manchester, United Kingdom, September 9-11, 2025.
12. Scientific machine learning for forecasting dynamical systems exhibiting deterministic chaos, **Invited talk**, Translational AI Center Seminar Series, Iowa State University, September 2, 2025.
13. Differentiable Physics: A physics-constrained and data-driven paradigm for scientific discovery, **Invited talk**, Johns Hopkins University and Indian Institute of Technology, Delhi Joint Seminar Series on Scientific Machine Learning, August 2025
14. Scientific machine learning for forecasting dynamical systems exhibiting deterministic chaos, **Invited talk**, Summer School: Scientific Machine Learning, Brin Mathematics Research Center, University of Maryland, August 2025.
15. SALSA-RL: Stability analyses in the latent space of actions for interpretable reinforcement learning, **Invited talk**, Frontiers in Scientific Machine Learning (FSML) Seminar Series, University of Michigan, July 11, 2025.
16. Predicting the long-term behavior of chaotic dynamical systems with scientific machine learning, **Invited talk**, CRM-IVADO Workshop on Accuracy and Efficiency in Scientific Machine Learning, Université de Montréal, June 2025.
17. The mean-squared-error is not enough: Improved prediction of chaotic dynamical systems with scientific machine learning, **Invited talk**, Statistical and Computational Challenges in Probabilistic Scientific Machine Learning (SciML), IMSI University of Chicago, June 2025.
18. Weather and Climate Emulation with physics-informed machine learning, **Invited Talk**, Verisk Extreme Event Solutions, June 4 2025.
19. Weather and Climate Emulation with physics-informed machine learning, **Invited Talk**, Seoul National University, May 19 2025.
20. The mean-squared-error is not enough: Improved prediction of chaotic dynamical systems with scientific machine learning, **Invited talk**, IUTAM Symposium on Machine Learning in Diverse Fluid Mechanics, Okinawa, May 16 2025.

21. Differentiable Physics: A physics-constrained and data-driven paradigm for scientific discovery, **Invited talk**, Inha University, Incheon, South Korea, May 2025.
22. Weather and Climate Emulation with State-of-the-Art Physics-Informed AI Algorithms, **Invited Talk**, Penn State Center for Socially Responsible Artificial Intelligence, April 9 2025.
23. Uncertainty quantification for scientific machine learning with joint neural architecture and hyperparameter search with DeepHyper, **Keynote talk**, NCAR Improving Scientific Software Conference, April 8 2025.
24. Turbulence closure modeling for large eddy simulations using differentiable physics, **Invited talk**, Oak Ridge National Laboratory CFD Webinar, March 27, 2025.
25. PDE-Constrained Learning of Data-Driven Turbulence Models, **Invited talk**, Thermal Transport Café, MIT, March 13, 2025.
26. Differentiable Physics: A physics-constrained and data-driven paradigm for scientific discovery, **Invited talk**, Penn State University Computational and Applied Mathematics Colloquium, Jan 27, 2025.
27. Non-intrusive reduced-order modeling with quantum reservoir computing, **Keynote talk**, IACM Digital Twins in Engineering and ECCOMAS Artificial Intelligence and Computational Methods in Applied Science, February 2025, Paris, France.
28. Deep-learning enhanced data assimilation for digital twins of high-dimensional complex dynamical systems, **Invited talk**, Korean Atomic Energy Research Institute (KAERI) Annual Workshop, January 22, 2025.
29. Uncertainty quantification for scientific machine learning with joint neural architecture and hyperparameter search with DeepHyper, **Invited talk**, Banff International Research Station workshop on Uncertainty Quantification in Neural Network Models, February 2025, Banff, Canada.
30. Neural ordinary differential equations for scientific machine learning, **Invited talk**, Param-Intelligence (PI) Seminar Series, Worcester Polytechnic Institute, November 7, 2024.
31. Scalable, adaptive, and explainable geometric deep learning with applications to computational physics, **Invited talk**, University of Illinois at Chicago, September 20, 2024.
32. PDE-constrained machine learning of data-driven closure models, **Invited talk**, Argonne National Laboratory, September 19, 2024.
33. Neural ordinary differential equations for scientific machine learning, **Invited talk**, AIGrid Hackathon, Rugen Island, Germany, September 12, 2024.
34. PDE-constrained machine learning of data-driven closure models, **Invited talk**, Society of Petroleum Engineering CFD Seminar, August 22, 2024.
35. Differentiable physics for closure modeling from data, **Invited talk**, Office of Naval Research Erosion Workshop, Johns Hopkins University, August 14, 2024.
36. Interpretable Fine-Tuning and Error Indication for Graph Neural Network Surrogate Models, US-ACM UQ-MLIP, Washington DC, August 13, 2024.
37. Interpretable SciML for fluid flows using multiscale graph neural networks, **Invited talk**, Healthy People and Healthy Planet Workshop, Imperial College, July 25, 2024.

38. Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics, **Invited talk**, Hong Kong University of Science and Technology Mechanical Engineering Seminar Series, April 17, 2024.
39. Differentiable physics for turbulence closure modeling from data, **Invited talk**, Unravel project meeting, University of Eindhoven, April 17, 2024.
40. Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics, **Guest lecture**, NUEN 689 "Deep Learning for Engineering Applications", Texas A & M University, April 9, 2024.
41. Differentiable physics for turbulence closure modeling from data, **Invited talk**, University of Maryland Numerical Analysis Seminar Series, April 2, 2024.
42. Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics, **Invited talk**, Fluid Dynamics Research Consortium Seminar Series, Pennsylvania State University, March 28, 2024.
43. Turbulence modeling for large-eddy simulations using neural differential equations, **Invited talk**, International Conference on Differential Equations for Data Science 2024 (DEDS2024), Feb 19-21, 2024.
44. Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics, **Invited talk**, Advanced Modeling and Simulations Seminar Series, University of Texas, El Paso, Feb 9, 2024.
45. On the construction of data-driven closures for large eddy simulations of turbulence, **Invited talk**, ERCOFTAC Workshop on Machine Learning for Fluid Dynamics, Sorbonne University, Paris, France, 6-8 March 2024.
46. Data assimilation with scientific machine learning, **Invited talk**, Indian Institute of Science, Education, and Research, Pune, December, 2023.
47. Anomaly detection for dynamical systems using Bayesian online changepoint detection, **Invited talk**, Brij Disa Center for Data Science and AI, Indian Institute of Management, Ahmedabad, December 2023.
48. Multiscale Graph Neural Network Architectures for Interpretable Scientific Machine Learning, **Invited talk**, Center for Mathematics and AI Seminar Series, George Mason University, October, 2023.
49. The research program of the Interdisciplinary Scientific Computing Laboratory, **Invited talk**, AI/ML Technical Group, Department of Aerospace Engineering, Pennsylvania State University, October, 2023.
50. Differentiable turbulence modeling, **Invited talk**, Aerospace Seminar Series, TU Delft, October, 2023.
51. Differentiable turbulence modeling, **Invited talk**, Autumn school on Scientific Machine Learning, CWI Amsterdam, October, 2023.
52. PythonFoam: In-situ data analyses with OpenFOAM and Python, MS 421.1, "Software Tools for Uncertainty Quantification and Machine Learning with Applications to Computational Science", 17th U.S. National Congress on Computational Mechanics, Albuquerque, 2023.
53. Multiscale Graph Neural Network Autoencoders for Interpretable Scientific Machine Learning, **Invited talk**, BIRS Scientific Machine Learning workshop, Banff International Research Station, June, 2023.

54. Neural architecture search for scientific machine learning, ICERM topical workshop on Mathematical and Scientific Machine Learning, Brown University, June, 2023.
55. Multiscale graph neural networks for scalable surrogate modeling of fluid dynamical systems, **Invited talk**, International Workshop on Reduced Order Methods, National University of Singapore, May, 2023.
56. Breaking boundaries: Why interdisciplinary research is key for tackling grand challenges, **Plenary talk**, Oklahoma State University, Mechanical and Aerospace Engineering Graduate Search Symposium, March 24, 2023.
57. A stabilized neural ordinary differential equation for scientific machine learning, **Invited talk**, SIAM Conference on Computational Science and Engineering, Amsterdam, 2023.
58. Neural architecture search for scientific machine learning, **Invited talk**, Rutgers Efficient AI Seminar Series, February, 2023.
59. Accelerating scientific discovery using physics-informed machine learning, **Invited talk**, Machine Learning for e-Science, Swedish e-Science Research Centre, November 30, 2022.
60. Efficient high-dimensional variational data assimilation with machine-learned reduced-order models, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2022.
61. A stabilized neural ordinary differential equation for scientific machine learning, **Invited talk**, SIAM Mathematics of Data Science, San Diego, September 28, 2022.
62. Neural forecasting of high-dimensional dynamical systems, **Invited talk**, University of Pittsburgh Computational Mathematics Seminar, September 20, 2022.
63. Quantifying Uncertainty in Deep Learning for Fluid Flow Reconstruction, USACM Thematic Conference on Uncertainty Quantification for Machine Learning Integrated Physics Modeling (MLIP), Crystal City, Virginia, August 18-19, 2022.
64. A stabilized neural ordinary differential equation for scientific machine learning, **Invited talk**, Arbonne Training Program on Exascale Computing (ATPESC), August 12, 2022.
65. Learning nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, 2022 AI + Science Summer School, University of Chicago, Data Sciences Institute, August 9, 2022.
66. Non-intrusive reduced-order modeling using scientific machine learning, **Invited talk**, Summer School on Reduced Order Methods in CFD, SISSA Trieste, July 13, 2022.
67. Learning nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, Accurate ROMs for Industrial Applications, Virginia Tech, July 7, 2022.
68. Learning nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, Brown University CRUNCH Seminar series, May 27, 2022.
69. Simple, low-cost and accurate data-driven geophysical forecasting with learned kernels, **Invited talk**, SIAM UQ, Atlanta, Georgia, April 12, 2022.
70. Reduced-order modeling of high-dimensional dynamical systems using scientific machine learning, **Invited talk**, IBiM Seminar Series, March 2022.
71. Emulating nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, APS March Meetings, March 14, 2022.

72. Reduced-order modeling of high-dimensional dynamical systems using scientific machine learning, **Invited talk**, National University of Singapore, Department of Mechanical Engineering, Distinguished Seminar Series, February 10, 2022.
73. Emulating complex systems from data using scientific machine learning, **Invited talk**, North Carolina State University, Department of Mathematics, February 1, 2022.
74. Research at the intersection of mathematics, computation, and data, **Invited talk**, BIT Mesra Alumni Association North America Faculty Webinar, January 29, 2022.
75. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, University of Waterloo, Department of Applied Mathematics, January 18, 2022.
76. Research at the intersection of mathematics, computation, and data, **Invited talk**, Physics & Engineering speaker series, North Park University, November 17, 2021.
77. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, 2021 CBE Computing Seminar Series, University of Wisconsin-Madison, October 22, 2021.
78. Parallelized emulator discovery and uncertainty quantification using DeepHyper, Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology, September 26-29, 2021.
79. Modified neural ordinary differential equations for stable learning of chaotic dynamics, **Invited talk**, Applied Mathematics Seminar Series, Texas Tech University, September 1, 2021.
80. Neural architecture search for surrogate modeling, **Invited talk**, ML4I Forum, Lawrence Livermore National Laboratory, August 10-12, 2021.
81. Scalable scientific machine learning for computational fluid dynamics, **Plenary talk**, ECCOMAS Thematic Conference on Computational Sciences and AI in Industry, June 7-9, 2021.
82. Neural architecture search for surrogate modeling, **Invited talk**, Data-driven Physical Sciences Seminar Series, Lawrence Livermore National Laboratory, May 27, 2021.
83. Incorporating inductive biases for the surrogate modeling of dynamical systems, **Invited talk** at Machine Learning for Dynamical Systems Special Interest Group, Alan Turing Institute, Imperial College London, April 14, 2021.
84. Surrogate modeling with learned kernels (Kernel Flows), **Invited talk**, Uncertainty Quantification in Climate Science, NASA JPL Climate Center Virtual Workshop, March 24, 2021.
85. Scalable recurrent neural architecture search for geophysical emulation, **Invited talk** at SIAM-CSE Minisymposium on Physics-Guided Machine Learning and Data-Driven Methods in Computational Geoscience, 2021.
86. Incorporating Inductive Biases as Hard Constraints for Scientific Machine Learning, **Invited talk**, MCS-LANS seminar, Argonne National Laboratory, February 2021.
87. Scalable scientific machine learning for computational fluid dynamics, **Invited talk**, Department of Mechanical Engineering, The City College of New York, October, 2020.
88. Data-driven model order reduction for geophysical emulation. **Invited talk** at the Second Symposium on Machine Learning and Dynamical Systems, Fields Institute, Toronto, September, 2020.
89. Scalable scientific machine learning for computational fluid dynamics, **Invited talk**, Department of Mechanical Engineering, Rice University, September, 2020.

90. Machine Learning Enablers for System Optimization and Design, **Invited talk**, MCS-LANS seminar, Argonne National Laboratory, August 2020.
91. Non-intrusive reduced-order model search for geophysical emulation, **Invited Lecture**, MAE259a: Data science for fluid dynamics (offered by Kunihiko Taira), University of California Los Angeles, June 2020.
92. Spatiotemporally dynamic implicit large eddy simulation using machine learning classifiers, Session on Domain-Aware, Interpretable and Robust Scientific Machine Learning Methods Applied to Computational Mechanics, AIAA Aviation Forum, June, 2020, Reno.
93. Machine learning for computational fluid dynamics, **Invited talk** at PyData Meetup Chicago, May 2020.
94. Recurrent neural architecture search for geophysical emulation using DeepHyper, **Invited talk** at AI-HPC seminar, Argonne National Laboratory, April, 2020.
95. Machine Learned Reduced-Order Models for Advective Partial Differential Equations, **Invited talk**, MCS-LANS seminar, Argonne National Laboratory, February, 2020.
96. Machine Learned Reduced-Order Models for Advective Partial Differential Equations, **Invited talk**, 2020 Spring Multiscale Seminar, Illinois Institute of Technology, Chicago, February, 2020.
97. General-purpose data science for general-purpose CFD: Integrating Tensorflow into OpenFOAM at scale, Workshop for Machine Learning for Transport Phenomena, February, 2020, Dallas.
98. Machine learning of sequential data for non-intrusive reduced-order models, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2019.
99. Tackling the limitations of conventional ROMs for advection-dominated nonlinear dynamical systems using machine learning, **Invited talk**, Advanced Statistics meets Machine Learning-III workshop, Argonne National Laboratory, November, 2019.
100. Data-driven sub-grid models for the large-eddy simulation of turbulence, **Invited talk**, John Zink Hamworthy Combustion, Tulsa, August, 2019.
101. Data-driven deconvolution for the sub-grid modeling of large eddy simulations of two-dimensional turbulence, **Invited talk**, SIAM-CSE, March, 2019.
102. Data-driven deconvolution for the large eddy simulation of Kraichnan turbulence, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2018.
103. A computational investigation of the effect of ground clearance in vertical ducting systems, 2018, Purdue University, Herrick Labs Conferences, July, 2018.
104. A neural network approach for the blind deconvolution of turbulent flows, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2017.
105. A generalized wavelet-based grid-adaptive and scale-selective implementation of WENO schemes for conservation laws, Texas Applied Mathematics and Engineering Symposium, The University of Texas, Austin, September 2017.
106. An explicit filtering framework based on Perona-Malik anisotropic diffusion for shock capturing and subgrid scale modeling of Burgers' turbulence, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2016.
107. A dynamic hybrid subgrid-scale modeling framework for large eddy simulations, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2016.

## Professional service

### *Program/Workshop committees and Funding Panels*

PythonFOAM Workshop Lead Organizer (<https://www.alcf.anl.gov/events/alcf-pythonfoam-workshop>).

DOE HPC program reviewer (INCITE, ADSP, ATPESC) - Various editions.

International Conference on Parallel Processing, Chicago, 2021.

Workshop Machine Learning for Fluid Dynamics, Amsterdam, 2026.

Wilkinson Postdoctoral Fellowship Committee, MCS Division, Argonne National Laboratory, 2022.

DOE AI for Earth System Predictability workshop session chair for neural networks.

Reviewer/Panelist - NSF-CISE, NASA-ESI, ARO-Multiscale Information Fusion, DOE FES/ASCR/SCGSR, Penn State ICDS Internal Funding.

### *Tutorials organized*

Tutorial lead - Scientific Machine Learning, Texas A & M University Institute of Data Science, November 2024.

Tutorial lead - Autoencoders for PDE surrogate models, ATPESC 2020.

Tutorial lead - Statistical methods for machine learning, ALCF AI4Science tutorial 2019, Argonne National Laboratory.

Tutorial lead - DeepHyper for scalable hyperparameter and neural architecture search on ALCF machines, ALCF Simulation Data and Learning workshop 2019, Argonne National Laboratory.

TensorFlow workshop, Mechanical & Aerospace Engineering, Oklahoma State University, 2018.

An introduction to high performance computing for middle school kids, National Lab Day, Oklahoma State University 2017, 2018.

### *Minisymposia*

MS Organizer & Session chair - SIAM CSE/UQ, AIAA Aviation, USNCCM, ECCOMAS (various editions).

Session chair - MAE Graduate Research Symposium, Oklahoma State University, 2018.

### *Journal Review*

Editor - Results in Engineering, Elsevier.

Journal reviewer for - AIAA Journal, Applied Mathematical Modeling, Chaos, Computer Methods in Applied Mathematics and Engineering, Communications in Computational Physics, Computers and Fluids, Computer Physics Communications, International Journal of Computational Fluid Dynamics, IEEE Transactions on Plasma Science, Journal of Fluid Mechanics, Journal of Scientific Computing, Physics of Fluids, Physica D, International Journal of Numerical Methods in Fluids, Journal of Computational Physics, Journal of Nonlinear Science, Nature Communications, Nature Machine Intelligence, Nature Scientific Reports, Theoretical and Computational Fluid Dynamics, Atmospheric Science Letters, New Journal of Physics, Transactions of Machine Learning Research, Machine Learning Science and Technology, Neurips, ICLR.

Guest Editor - Special issue on Scientific Machine Learning - Mechanics Research Communications.

## Software developed

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